THEORY FOR DECOUPLING IN HIGH-T$_{\rm c}$ SUPERCONDUCTORS FROM AN ANALYSIS OF THE LAYERED XY MODEL WITH FRUSTRATION

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Abstract

The nature of decoupling in the mixed phase of extremely type-II layered superconductors is studied theoretically through a duality transformation of the layered XY model with frustration. In the limit of weak coupling, we generally find that the Josephson effect is absent if and only if the phase correlations within isolated layers are short range. In the case specific to uniform frustration, we notably identify a decoupled pancake vortex liquid phase that is bounded by first-order and second-order decoupling lines in the magnetic field vs. temperature plane. These transitions potentially account for the flux-lattice melting and for the flux-lattice depinning that is observed in clean high-temperature superconductors.

Introduction. High-T_c superconductors are perhaps the best known example of an extremely type-II layered superconductor.[1] The vortex lattice that exists in the mixed phase of clean oxide superconductors melts through a first-order transition for magnetic fields applied perpendicular to the layers.[2] The first-order line, $H_\perp = H_m(T)$, begins at the zero-field critical point, T_c, but it ends strangely in the middle of the phase diagram. The depinning line $T = T_{dp}(H_\perp)$, which marks the point at which the flux lattice depins itself through thermal excitations, appears to be independent of this melting line.[3,4] The first-order transition is commonly interpreted as either a vortex lattice melting transition,[1] or as a layer decoupling transition.[5,6] The respective theoretical approaches have been primarily based on elastic medium descriptions of the vortex matter that notably omit topological defect excitations.[7,8] These theories also fail to account for the multicritical point mentioned above in the absence of disorder.[9]

In this paper, we shall model the thermodynamics of the interior of the mixed phase in extremely type-II anisotropic superconductors by the layered XY model with uniform frustration.[10-12] The nature of the Josephson effect between layers is uncovered through a *partial* duality analysis of the XY model.[13-17] A subsequent weak-coupling analysis at high perpendicular fields yields a low-temperature phase made up of coupled 2D vortex lattices that is separated from a decoupled liquid of planar vortices at high temperatures by a second order melting line. It is further argued that the decoupled liquid phase experiences a first-order phase transition into a coupled solid phase as the perpendicular field is lowered into the strong-coupling regime.[16,17] The phase diagram that results (see Fig. 1) is compared with recent experimental reports of multicritical phenomena in the mixed phase of high-temperature superconductors.[3,4]

Layered XY Model. Before considering the uniformly frustrated case that describes the mixed phase of extremely type-II superconductors, let us first perform a duality analysis of the layered XY model without frustration.[18] The corresponding energy functional reads

$$E_{XY}^{(3)} = -J_\parallel \sum_{l=1}^{N} \sum_{\vec{r}} \sum_{\mu=x,y} \cos[\Delta_\mu \phi(\vec{r}, l) - A_\mu(\vec{r}, l)]$$
$$- J_\perp \sum_{l=1}^{N-1} \sum_{\vec{r}} \cos[\phi(\vec{r}, l+1) - \phi(\vec{r}, l) - A_z(\vec{r}, l)], \qquad (1)$$

where $\phi(\vec{r}, l)$ is the superconducting phase at a point $\vec{r}$ in layer l. Above , Δ_μ denotes the

nearest-neighbor difference operator along the $\hat{\mu}$ direction, while A_μ represents a purely longitudinal vector potential. The Josephson penetration length $\gamma' a$ provides a natural scale for the model (1) in the limit of weak inter-layer coupling, in which case the model anisotropy parameter $\gamma' = (J_\parallel/J_\perp)^{1/2}$ is much larger than unity. Here, a denotes the (square) lattice constant for each layer. Last, any generalized phase auto-correlation function set by an integer source field, $p(r)$, is related to the corresponding partition function

$$Z_{XY}^{(3)}[p] = \int \mathcal{D}\phi \, e^{-E_{XY}^{(3)}/k_B T} e^{i \sum p\phi} \tag{2}$$

by the quotient

$$\left\langle \exp\left[i \sum_r p(r)\phi(r)\right]\right\rangle = Z_{XY}^{(3)}[p]/Z_{XY}^{(3)}[0]. \tag{3}$$

We shall now employ the well-known dual representation[13] of the XY model (1) based on the Fourier series expansion $e^{\beta \cos\theta} = \sum_{n=-\infty}^{\infty} I_{|n|}(\beta)e^{in\theta}$ of the Gibbs distribution in terms of modified Bessel functions, $I_n(x)$. This identity allows the phase variables to be integrated out of (2). Resummation over the parallel link fields n_x and n_y then yields the form

$$Z_{XY}^{(3)}[p] = I_0^{\mathcal{N}'}(\beta_\perp) \cdot Z_{\mathrm{CG}}[p] \cdot \Pi_{l=1}^N Z_{XY}^{(2)}[0] \tag{4}$$

for the partition function of the layered XY model in terms of a product of a layered Coulomb gas ensemble (CGE)

$$Z_{\mathrm{CG}}[p] = \sum_{\{n_z(r)\}} y_0^{N[n_z]} \cdot \Pi_{l=1}^N C_l[q_l] \cdot e^{-i \sum_r n_z A_z} \tag{5}$$

with N isolated XY model layers ($J_\perp = 0$).[17] Above, $n_z(r)$ is the remaining integer link field between adjacent layers that is effectively restricted to take values $n_z(r) = 0, \pm 1$ in the weak-coupling limit $J_\perp \ll k_B T$. Indeed, each configuration in the CGE (5) is weighted by the bare fugacity $y_0 = J_\perp/2k_B T$ raised to the power $N[n_z] \cong \sum_{\vec{r},l} |n_z(\vec{r},l)|$ equal to the total number of n_z-charges. The latter so-called fluxons physically represent vortex rings in between adjacent layers.[14] Each configuration is further weighted by a product of generalized auto-correlation functions $C_l[q_l] = \left\langle \exp\left[i \sum_{\vec{r}} q_l(\vec{r})\phi(\vec{r},l)\right]\right\rangle_{J_\perp=0}$ over each layer l in isolation that are evaluated at sources $q_l(\vec{r}) = p(\vec{r},l) + n_z(\vec{r},l-1) - n_z(\vec{r},l)$. Last, we have the parameters $\beta_{\parallel,\perp} = J_{\parallel,\perp}/k_B T$, while $\mathcal{N}'$ denotes the total number of rungs between layers.

3

To proceed further, it is instructive to consider a single neutral pair of unit n_z charges that lie in between layers l' and $l' + 1$ in the absence of an external source, $p = 0$, with the negative and positive charges located at planar sites $\vec{r}_1$ and $\vec{r}_2$, respectively. The gauge-invariant product over intra-layer autocorrelation functions in the layered CGE (5) then reduces to the product $|C_{l'}(\vec{r}_1 - \vec{r}_2)| \cdot |C_{l'+1}(\vec{r}_1 - \vec{r}_2)|$ of the corresponding phase autocorrelation functions,

$$C_l(\vec{r}_1, \vec{r}_2) = \left\langle \exp\left[i\phi(\vec{r}_1, l) - i\phi(\vec{r}_2, l) \right] \right\rangle_{J_\perp = 0}, \tag{6}$$

within isolated layers. This function varies algebraicly with the separation as

$$|C_l(\vec{r})| = g_0 (r_0/|\vec{r}|)^{\eta_{2D}} \quad \text{for} \quad |\vec{r}| \ll \xi_{\text{vx}}, \tag{7}$$

while it decays exponentially with the separation as

$$|C_l(\vec{r})| = g_0 \exp(-|\vec{r}|/\xi_{\text{vx}}) \quad \text{for} \quad |\vec{r}| \gg \xi_{\text{vx}}. \tag{8}$$

Here, $\eta_{2D} = \eta_{\text{sw}} + \eta_{\text{vx}}$ is the 2D correlation exponent inside layer l, where $\eta_{\text{sw}} = (2\pi\beta_\parallel)^{-1}$ and η_{vx} are the respective spin-wave and vortex contributions. Also, ξ_{vx} denotes the 2D phase correlation length, while the length $r_0 = a/(2^{3/2}e^\gamma)$ is set by Euler's constant, γ. The effective layered CGE (5) therefore takes the form

$$Z_{\text{CG}}[0] = \sum_{\{n_z\}} (g_0 y_0)^{N[n_z]} \exp\left\{ -\frac{1}{2} \sum_l \sum_{\vec{r}_1, \vec{r}_2} q_l(\vec{r}_1) \left[\eta_{2D} \ln(r_0/|\vec{r}_1 - \vec{r}_2|) - V_{\text{string}}^{[q_l]}(\vec{r}_1, \vec{r}_2) \right] q_l(\vec{r}_2) \right.$$
$$\left. - i \sum_l \sum_{\vec{r}} n_z(\vec{r}, l) A_z(\vec{r}, l) \right\} \tag{9}$$

in the limit of dilute fluxon (n_z) charges. At separations within a correlation length, $|\vec{r}_1 - \vec{r}_2| \ll \xi_{\text{vx}}$, the fluxons experience a pure Coulomb interaction ($V_{\text{string}}^{[q_l]} = 0$). At large separations $|\vec{r}_1 - \vec{r}_2| \gg \xi_{\text{vx}}$, on the other hand, the fluxons experience a pure ($\eta_{2D} = 0$) confining interaction $V_{\text{string}}^{[q_l]}(\vec{r}_1, \vec{r}_2) = |\vec{r}_1 - \vec{r}_2|/\xi_{\text{vx}}$ between those points $\vec{r}_1$ and $\vec{r}_2$ in layer l that are connected by a string [see Eq. (8) and ref. [19]]. Below, we determine the thermodynamic nature of the superconducting and "normal" phases that correspond to Eqs. (7) and (8), respectively.

Consider first the case where (quasi) long-range intra-layer phase correlations are present: $\xi_{\text{vx}} = \infty$ and $V_{\text{string}}^{[q_l]} = 0$. Summing independently over charge configurations of

the CGE (9) that are restricted to take values $n_z = 0, \pm 1$ at each site plus an appropriate Hubbard-Stratonovich transformation[12] yields an equivalent renormalized Lawrence-Doniach (LD) model[1] set by the continuum energy functional

$$E_{\text{LD}} = \bar{J}_\parallel \int d^2r \left[\sum_{l=1}^{N} \frac{1}{2} (\vec{\nabla}\theta_l)^2 - \Lambda_0^{-2} \sum_{l=1}^{N-1} \cos(\theta_{l+1} - \theta_l - A_z) \right]. \tag{10}$$

Here, $\bar{J}_\parallel = k_B T / 2\pi \eta_{2D}$ is the macroscopic phase rigidity of an isolated layer,[20] while $\Lambda_0 = a(\bar{J}_\parallel / g_0 J_\perp)^{1/2}$ is the renormalized Josephson scale. The above continuum description (10) is understood to have an ultra-violet cut-off on the order of the lattice constant, $r_0 \sim a$. Eq. (10) is known to sustain a macroscopic Josephson effect at temperatures below $k_B T_* \cong 4\pi \bar{J}_\parallel$.[14,15] Also, the factorization (4) plus the continuum limit (10) indicate the expression

$$\langle \cos \phi_{l,l+1} \rangle \cong \frac{1}{2} \beta_\perp + f_0 \left(\frac{r_0}{\Lambda_{\text{J}}} \right)^\eta \tag{11}$$

for the local Josephson coupling, where $\phi_{l,l+1}(\vec{r}) = \phi(\vec{r}, l+1) - \phi(\vec{r}, l) - A_z(\vec{r})$ is the gauge-invariant phase difference between consecutive layers. An analysis of the double-layer case yields an effective anisotropy scale $\Lambda_{\text{J}} = \Lambda_0 / 2^{1/2}$ and the limiting values $\eta \to \eta_{2D}$ and $f_0 \to g_0$ for the exponent and for the prefactor at low temperatures, $\eta_{2D} \ll 1$ (see ref. [17]). Expression (11) indicates that a crossover to strong coupling, $\langle \cos \phi_{l,l+1} \rangle \sim 1$, must therefore take place in the isotropic regime $a \sim \Lambda_0$ and/or at a temperature of order the Josephson scale $T_{\text{J}} = J_\perp / k_B$.

Consider next the case in which intra-layer correlations are short range: $\xi_{\text{vx}} < \infty$. Inter-layer fluxon (n_z) pairs are then bound by a confining string (8). Application of the CGE (5) yields Koshelev's formula[11]

$$\langle e^{i\phi_{l,l+1}} \rangle \cong y_0 \int d^2r |C_l(r)| \cdot |C_{l+1}(r)|/a^2 \tag{12}$$

for the local Josephson coupling in this decoupled phase (see ref. [17]). Substitution of the form (8) for the short-range intra-layer autocorrelator in turn yields the explicit formula

$$\langle \cos \phi_{l,l+1} \rangle \cong \frac{\pi g_0^2}{4} \left(\frac{\xi_{\text{vx}}}{a} \right)^2 \beta_\perp \tag{13}$$

for the local Josephson coupling. It can be shown that the macroscopic Josephson effect is absent in this decoupled phase.[16,17]

We can now determine the phase diagram of the layered XY model.[18] It is well known that an isolated XY layer looses phase coherence above a temperature $k_B T_c^{(2D)} \cong \frac{\pi}{2} J_{\parallel}$.[13] The transition is driven by the unbinding of vortex/anti-vortex pairs and it is second-order.[21] Consider first the weak-coupling limit $\langle \cos \phi_{l,l+1} \rangle \to 0$. By the previous analysis, we then conclude that the layers are Josephson coupled at low temperature $T < T_c^{(2D)}$ following the renormalized LD model (10), while they are decoupled at high temperature $T > T_c^{(2D)}$. Eq. (13) indicates, also, that the selective high-temperature expansion breaks down ($\langle \cos \phi_{l,l+1} \rangle \sim 1$) in the decoupled phase at a temperature $T_{\times}$ set by the identification of length scales $\Lambda_0 \sim \xi_{vx}(T_{\times})$. The second-order transition therefore takes place at a temperature T_c that lies inside of the dimensional crossover window $T_c^{(2D)} < T < T_{\times}$ for large yet finite anisotropies $\gamma' \gg 1$. These conclusions agree with what is presently understood for the layered XY model.[18]

Uniformly Frustrated Case. Consider now the layered XY model (1) in the presence of a uniform frustration, $A_{\mu} = (0, b_{\perp} x, 0)$, which describes the mixed phase of an extremely type-II superconductor in a field $B_{\perp} = (\Phi_0/2\pi a) b_{\perp}$ aligned perpendicular to the layers.[10-12] The duality analysis just performed can then be repeated wholesale, yet with the following modifications:[16,17] (*a*) Each isolated XY layer now undergoes a 2D melting transition that is mediated by the unbinding of dislocation pairs[21] at a temperature[22] $k_B T_m^{(2D)} \cong J_{\parallel}/20$, while (*b*) the ultra-violet cut-off, r_0, of the renormalized LD model (10) is now of order the average spacing between planar vortices, $a_{vx} = (\Phi_0/B_{\perp})^{1/2}$. (The CGE [Eqs. (7)-(9)] must be coarse-grained up to the new ultra-violet scale, a_{vx}.) In the weak-coupling limit $\langle \cos \phi_{l,l+1} \rangle \to 0$ reached at high fields $B_{\perp} \gg B_{\perp}^* = \Phi_0/\Lambda_0^2$, we therefore have N 2D vortex lattices that show a macroscopic Josephson effect at low temperatures $T < T_m^{(2D)}$, while a decoupled liquid of planar vortices exists at high temperatures $T > T_m^{(2D)}$. At large yet finite anisotropies, $\gamma' \gg 1$, it is useful once again to determine the temperature scale $T_{\times}$ at which point the selective high-temperature expansion (13) for the local Josephson coupling breaks down. This again takes place roughly when Λ_0 and ξ_{vx} are comparable. As in the previous case without frustration, we therefore expect a second-order melting transition at a temperature T_m that lies inside the dimensional crossover window[18] $T_m^{(2D)} < T < T_{\times}$.

Yet what happens when the local Josephson coupling $\langle \cos \phi_{l,l+1} \rangle$ approaches unity as

the field $B_\perp$ is lowered? It is useful to first define a decoupling contour

$$\langle \cos \phi_{l,l+1} \rangle = \langle \cos \phi_{l,l+1} \rangle_D, \qquad (14)$$

in the T-$B_\perp$ plane. Numerical simulations indicate that $\langle \cos \phi_{l,l+1} \rangle_D$ is a constant less than but of order unity.[11] The result (11) for the local Josephson coupling in the coupled phase yields (i) a contour line at temperatures of order the Josephson energy, $k_B T_{\rm J} = J_\perp$, for high perpendicular fields $B_\perp \gg B_\perp^*$, and (ii) a contour line at perpendicular fields of order $B_\perp^*$ for temperatures near $T_m^{(2D)}$. Since no phase transition is possible in the screened CGE (9) that describes the coupled phase, this contour line must therefore represent a crossover into a flux-line lattice regime that exists at lower temperatures and fields. At high temperatures $T > T_\times$ inside the weak-coupling regime of the decoupled phase, the string interaction (8) binds together fluxon-antifluxon pairs into stable dipoles of dimension $\xi_{\rm vx}$ that do not overlap. It can be shown that such fluxon pairs begin to overlap and dissociate in the vicinity of the decoupling contour (14) for temperatures that lie outside of the 2D critical regime ($\xi_{\rm vx} \sim a_{\rm vx}$).[17] We therefore expect a first-order transition along this line due to the absence of a nearby divergent length scale.

The above results are summarized by the schematic phase diagram shown in Fig. 1. The phenomenology $J_\perp \propto (T_c - T)/T_c$ for the Josephson energy in the vicinity of the zero-field transition at T_c yields the same linear temperature dependence for the first-order decoupling field,[2,5,6] $H_D(T)$ [see Eqs. (13) and (14)]. Eq. (11) also implies that the decoupling contour (14) continues into the coupled phase at temperatures $T < T_m$, there representing a crossover. The first-order line (14) must therefore *end* at the second-order melting line, $T = T_m$. The melting curve then continues up in field along the latter second-order line. Finally, it is possible that a vestige of the second-order melting transition at high fields $B_\perp > B_\perp^*$ persists down into the low-field region in the form of a crossover (see Fig. 1).

Discussion. The first-order flux-lattice melting line in clean high-temperature superconductors is experimentally observed to end at a multi-critical point.[2,3] The phase diagram proposed in Fig. 1 for the mixed phase of extremely type-II layered superconductors also exhibits a multicritical point at a temperature and field $T_0 \sim T_m^{(2D)}$ and $B_0 \sim B_\perp^*$. This point agrees qualitatively with the high-T_c phase diagram.[2,5] Also, bulk pinning is observed to become relatively strong in clean oxide superconductors at low temperatures

and high fields, $T < T_m^{(2D)}$ and $H_\perp > B_\perp^*$.[3] The quasi-2D vortex lattice phase that is identified in Fig. 1 coincides with this regime. It is a smectic (super) solid,[8] and it can thus adjust better to a random landscape of point pins than a rigid vortex lattice. Recent observations of muon spin resonance in the mixed phase of clean high-temperature superconductors are consistent with such a picture of enhanced point pinning due to dimensional crossover.[23] We remind the reader that all effects due to magnetic screening[24] have been completely neglected in the present theory.

In conclusion, the phase diagram proposed in Fig. 1 for the layered XY model with uniform frustration is strikingly similar to that of the mixed phase in high-T_c superconductors.[2,3] It is perhaps more important to point out, however, that the above duality analysis yields only *two* thermodynamic phases at weak coupling: a coupled superconductor (7) and a decoupled "normal" state (8). This indicates that neither the Friedel scenario (decoupled superconducting layers) nor the flux-line liquid state (coupled normal layers) are thermodynamically possible in the absence of disorder.[1]

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Figure Caption

Fig. 1. Shown is a schematic phase diagram for the uniformly frustrated XY model (1) made up of a finite number of weakly-coupled layers. The cross-over transition that is represented by the horizontal dashed line at low temperatures $T_{\text{J}} < T < T_m^{(2D)}$ is broad (see ref. [17]).

(NO BULK PINNING)

$H_\perp$

H_{c2}

$B^\times$

COUPLED
2D VORTEX
LATTICES

DECOUPLED
PANCAKE
VORTEX
LIQUID

2D-3D CROSSOVER

FIRST-ORDER
SECOND-ORDER
CROSS-OVER

B^*

FLUX-LINE
LATTICE

DEFECTIVE
FLUX-LINE LATTICE

0 T_J $T_m^{(2D)}$ T_c